

Topological properties of a Valence-Bond-Solid

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Abstract. We present a projector quantum Monte Carlo study of the topological properties of the valence-bond-solid ground state in the J - Q_3 spin model on the square lattice. The winding number is a topological number counting the number of domain walls in the system and is a good quantum number in the thermodynamic limit. We study the finite-size behavior and obtain the domain wall energy density for a topological nontrivial valence-bond-solid state.

1. Introduction

While topological order has mainly been discussed in the context of exotic states such as quantum spin liquids [1, 2], similar topological quantum numbers can also arise in systems with long-range order. The simplest example of a topological quantum number is the winding number of a dimer model [3]. In the classical close-packed dimer model on the square lattice (as an example of a simple bipartite lattice), a winding number $W = (w_x, w_y)$ can be defined by assigning a directionality (arrow) from sublattice A to sublattice B for each dimer. Superimposing any such configuration of arrows onto two reference configurations (conventionally one with the dimers forming horizontal or vertical columns), closed loops are formed and the winding numbers correspond to the total x and y currents normalized by the system length L [3].

In the quantum dimer model (QDM), the classical dimer configurations are the basis states. For $S = 1/2$ quantum spins on a bipartite lattice, any total spin singlet can be expanded in Valence-bond states (VBs) with positive-defined expansion coefficients. The VBs are dimers with the added spin-singlet internal structure and the configurations can again be classified according to the winding number [4]. Since the Hamiltonian of the QDM contains only local operators that have no matrix element between states of different winding numbers, the Hilbert space can be divided into different winding number sectors, i.e., the topological winding number is a good quantum number. However, for general VB states, longer bonds are introduced, which makes the bond operators in the Hamiltonian non-local. For finite size systems, the winding number can be changed if bonds of lengths exceeding $1/4$ of the system length appear. Therefore, the winding number can only be conserved in the thermodynamic limit.

To investigate the emergent conserved winding number in an $S = 1/2$ spin system, we here study the J - Q_3 Model on the square lattice [5]. The Hamiltonian of the model is

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q_3 \sum_{\langle ij, kl, mn \rangle} C_{ij} C_{kl} C_{mn} \quad (1)$$

with $C_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$ recognized as a singlet projector. The J term of H is the standard Heisenberg exchange and the Q_3 terms have the singlet projectors arranged in columns, as shown in Fig. 1(a). This model hosts a columnar valence-bond solid (VBS) ground state when Q_3/J is sufficiently large [6]. Ignoring quantum fluctuations, the VBS ground state is sketched as an ordered VBS breaking the Z_4 symmetry of the Hamiltonian, as shown in Fig. 1(b). As previously studied in the context of QDMs [7], a VBS with domain walls on a periodic lattice corresponds to a non-zero winding number—a case of $W = (1, 0)$ is shown in Fig. 1(c).

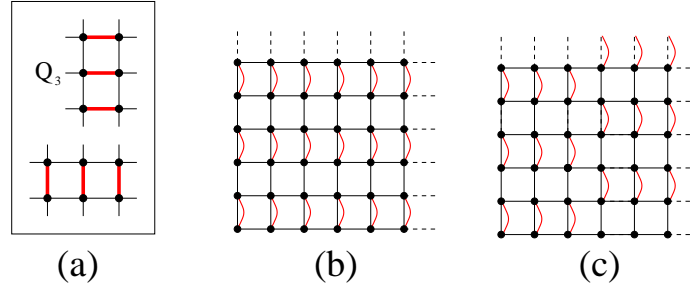


Figure 1. Illustrations of (a) the Q_3 terms, (b) the columnar VBS state, and (c) a VBS state with winding number $W = (1, 0)$ (on a periodic lattice).

In this paper, we consider the pure Q_3 model without any J term to study the VBS ground state. We will demonstrate explicitly, using projector quantum Monte Carlo (PQMC) calculations, that there is an emergent topological quantum number (a winding number) associated with the VBS order in the thermodynamic limit, while in a finite system the winding number is not conserved. In this case the topological sectors correspond to different types of domain walls, which are unstable (non-conserved) in finite systems but become stable in the thermodynamic limit.

2. Projector Quantum Monte Carlo method

The model with $Q_3 > 0$ in (1) does not have sign problems. We thus take advantage of the PQMC method with efficient loop update algorithms [8, 9, 10] to study the model. The method is based on applying a high power of the Hamiltonian to a trial state $|\psi_0\rangle$,

$$|\psi_m\rangle = (-H)^m |\psi_0\rangle. \quad (2)$$

For sufficient large m , $|\psi_m\rangle$ approaches the ground state $|0\rangle$ of the model. As the ground state $|0\rangle$ of a bipartite J - Q_3 model is guaranteed to be a total spin singlet, it is particularly convenient to use a trial state expanded in the VB basis $|V_r\rangle$ in the singlet sector. Then only the singlet sector is considered from the outset, leading to faster convergence with m .

The energy of the projected state can be calculated in the following way [11]

$$E = \frac{\langle N | H | \psi_m \rangle}{\langle N | \psi_m \rangle} = - \frac{\langle N | (-H) (-H)^m | \psi_0 \rangle}{\langle N | (-H)^m | \psi_0 \rangle}, \quad (3)$$

where $|N\rangle$ is one of the Néel states in the z -spin basis, which has equal overlap with all VBs.

By writing $(-H)^m$ as a sum over all possible strings of the individual Q_3 terms in Eq. (1), the above expression is evaluated by implementing importance sampling of the operator strings with the efficient loop algorithm [9, 10]. The implementation of the algorithm to the J - Q_3 Hamiltonian has been described briefly in [12]. In the end, the energy E is calculated as $E = -\langle n_d + n_f/2 \rangle$ with n_f the number of bond flips and n_d the number of diagonal operations.

3. Results

We chose a basis state $|\psi_0\rangle = |V_r\rangle$ as the trial state and consider the cases that $|V_r\rangle$ in different winding number sectors W . The detailed definition of the winding number of a VB state can be found, e.g., in Refs. [3, 2]. In the PQMC simulations, besides the energy, we also sample the probability, $P(W)$, of a projected state in the topological sector $W = (w_x, w_y)$. This is done by calculating the winding number of each projected VBs $P_k|V_r\rangle$, with P_k a operator string with length m generated in the MC processes.

In the case that the trial state is a VBs in the winding number sector $W = (0,0)$, the ground columnar VBS state will be projected out quickly, i.e., within a small m/N , which can be defined as a projecting "time" (closely related to imaginary time [13]). This is indicated by the convergence of the ground state energy density $e_0(L)$ for a system with linear size L .

Now turn to the cases that the trial state is in the nontrivial winding number sector $W \neq (0,0)$. For small systems, the columnar VBS state is again projected out after some projection time m/N . This is indicated by the convergence of the energy density $e(L)$ to the ground state value $e_0(L)$. Meanwhile, the probability $P(W)$ decreases (to 0 for $L \rightarrow \infty$). However, as the system size increases, the projection time m/N needs to grow as well in order for the ground state to be obtained. In the thermodynamic limit, we expect that the system will stay in the sector with the initial winding number W , and then it is also plausible that the energy of the system will converges to a value $e_W > e_0$ corresponding to the lowest excited state within the sector W .

To demonstrate such behavior, we introduce the energy density $e_W(L)$ of states in the winding number sector W , which is obtained by only sampling those states in the sector W . Figure 2 shows the "time evolution" of the probability $P(W)$ for the system staying in the original winding number sector $W = (0,0)$, $W = (1,0)$, and $W = (2,0)$ as a function of m/L^2 , respectively, for a system with linear size $L = 96$ (lower panel). The corresponding energy density $e_W(L)$ converges to the values which are higher than $e_0(L)$, if $W \neq 0$ (upper panel).

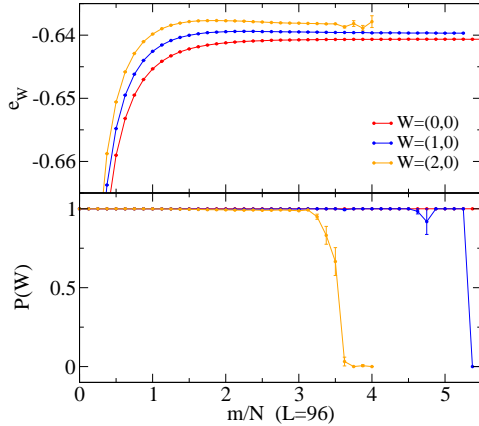


Figure 2. The probability $P(W)$ and the energy density $e_W(L)$ as functions of time m/N (projector power rescaled by the system volume).

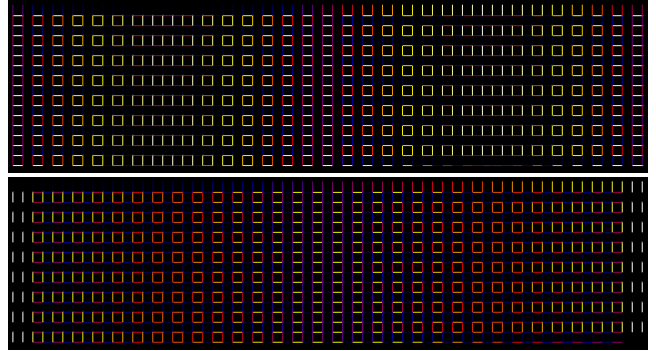


Figure 3. Snapshots of $\langle B_\alpha(\mathbf{r}) \rangle$ for a periodic system with winding number $W = (1,0)$, in which a 2π domain wall (four separate $\pi/2$ domain walls) is formed (upper panel) and for an open system with appropriate boundary conditions in which a π domain wall is forced (lower panel).

We now study the reason of the energy gap between a system in a nontrivial topological sector and in the $W = 0$ ground state. It is well known that the ground state of the $J-Q_3$ is the columnar VBS. The VBS state can be detected by the columnar VBS order parameter, which

is defined by the operators

$$D_x = \frac{1}{N} \sum_{x,y} B_{\hat{x}}(x,y)(-1)^x, \quad D_y = \frac{1}{N} \sum_{x,y} B_{\hat{y}}(x,y)(-1)^y. \quad (4)$$

where the dimer operator B_α is used:

$$B_\alpha(\mathbf{r}) = \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r} + \alpha) \quad (5)$$

where $\alpha = \hat{x}, \hat{y}$ denotes the lattice unit vector in the two directions. In a columnar VBS, either D_x or D_y has a nonzero expectation value.

However, if a state bears a nontrivial winding number, the lattice translational symmetry with period two is also broken. As an example, Fig. 3 (upper panel) shows a snapshot of the bond configuration $\langle B_\alpha(\mathbf{r}) \rangle$ for a projected state with winding number $W = (1, 0)$. To describe such a state, it is useful to define the local order parameters for the VBS state. Consider the case that there is still translational invariant VBS with period two along one axis of the square lattice, say y axis. The one-dimensional local x and y order parameters as a function of the x coordinate are defined [14] as follows:

$$D_x(x) = [\langle B_{\hat{x}}(x,y) \rangle - \frac{1}{2} \langle B_{\hat{x}}(x-1,y) \rangle - \frac{1}{2} \langle B_{\hat{x}}(x+1,y) \rangle] (-1)^x, \quad (6)$$

$$D_y(x) = [\langle B_{\hat{y}}(x,y) \rangle - \langle B_{\hat{y}}(x,y+1) \rangle] (-1)^y. \quad (7)$$

These two local order parameters are independent of the y coordinate. Following theoretical expectations [15], The VBS angle $\theta(x)$ can also be defined [14],

$$\theta(x) = \text{atan} \left[\frac{D_y(x) + D_y(x+1)}{2D_x(x)} \right], \quad (8)$$

such that $\theta = 0$ and $\theta = \pi$ for a fully x or y oriented VBS order, respectively.

To understand the energy gap between system in a nontrivial topological sector and in the $W = 0$ ground state, we first set asymmetric open boundary conditions on a $L \times L$ cylindrical lattice, where the x -direction boundaries have been modified. By removing Q_3 terms with vertical bonds closest to the left edge on every even row and closest to the right edge on every odd row, we obtain a state with forced VBS angle $\theta(0) = \pi/2$ and $\theta(L) = -\pi/2$. A snapshot of the bond strength $\langle B_\alpha(\mathbf{r}) \rangle$ for the state projected out from simple trial state with a corresponding domain wall is shown in Fig. 3 (lower panel). More properties of the projected state are shown in Fig. 4 (right), where the two local order parameters and the VBS angle are plotted as functions of x coordinate and various system sizes L . In this case, the local order parameter $D_x(x)$ is maximized in the center and goes to zero at boundaries; $D_y(x)$ is about 0.75 at the left boundary, but gradually changes to -0.75 at the right boundary. The VBS angle $\theta(x)$ changes from $\pi/2$ to $-\pi/2$. Clearly a domain wall is formed, as expected. According to the total change of the VBS angle, we define this as a π domain wall (which consist of two $\pi/2$ domain walls).

The energy density of the state with π domain wall $e_\pi(L)$ can be calculated as described above. The resulting $e_\pi(L)$ is larger than the ground state energy density $e_0(L)$ of a $L \times L$ cylindrical lattice with symmetric boundary modification (i.e., forcing a VBS with no domain wall). The energy difference is entirely due to the presence of the domain wall. We thus define the domain wall energy per unit length as

$$\kappa_\pi(L) = [e_\pi(L) - e_0(L)]L \quad (9)$$

As shown in Fig. 5, when system size goes to infinity, the domain wall energy per unit length converge to a constant κ_π , which is estimated as 0.434(9), as listed in Table 1.

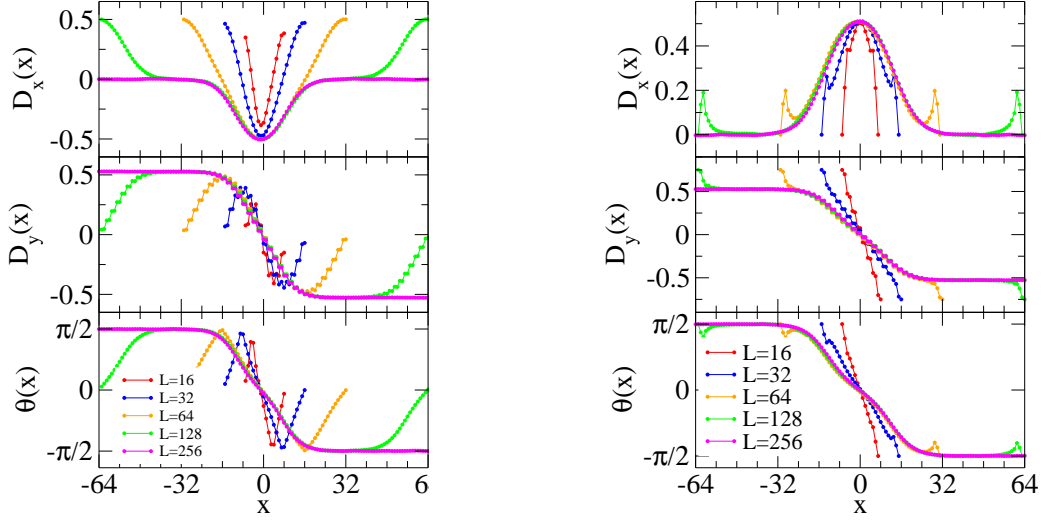


Figure 4. The local order parameters $D_x(x)$, $D_y(x)$ and the VBS angle $\theta(x)$ for projected states in the topological sector $W = (1,0)$ with periodic boundaries (left) and for the states with a π domain wall (right) in a system with asymmetric open boundaries.

Similarly, a $\pi/2$ domain wall can be realized by setting asymmetric open boundary conditions forcing horizontal and vertical bond patterns at the edges. The energy difference to $e_0(L)$ multiplied by the system size again converges to a constant when system size L tends to infinity (see Fig. 5). The constant is thus identified as the domain wall energy $\kappa_{\pi/2}$ for the $\pi/2$ domain wall with the estimated value being a half of the π domain wall energy, as listed in Tab. 1.

We now return to systems with periodic boundaries. In the case of large enough system, the projected energy eigenstate is still in the winding number sector W of the initial state. Take the $W = (1,0)$ case as an example. Figure 4 (left panel) shows the local order parameters and VBS angle as functions of the x coordinate. $D_x(x)$ has a minimum in the center and maxima at the left and right sides, while $D_y(x)$ is almost zero at the edges gradually grows to a maximum of 0.5, then decays to a minimum about -0.5 , and finally returns to 0. As the result, the VBS angle $\theta(x)$ changes from 0 to $\pi/2$, then to $-\pi/2$, and back to 0. Domain walls are clearly formed here and their dynamics in a large system is very slow and practically locked in to their locations in the initial state. According to the total change of the VBS angle we define this as a 2π domain wall (which can be regarded as four elementary $\pi/2$ domain walls). A finite-size scaling analysis of the energy density gap to the ground state ($W = 0$) $e_W(L) - e_0(L)$ multiplied by the system size L is shown in Fig. 5. Clearly, the scaled gap converges to a constant, which can be understood as the 2π domain wall energy per unit length $\kappa_{2\pi}$. The estimated $\kappa_{2\pi}$ is indeed twice that of the π domain wall, as seen in Table 1.

We further calculated the energy density gap $e_W(L) - e_0(L)$ from the projected state in the winding number sector $W = (2,0)$ to the ground state for several system sizes. The local order parameters and VBS angles as functions of the x -direction shows that there is a 4π domain wall. Again the energy gap multiplied by the system size converges to a constant, which is the 4π domain wall energy. The estimated domain wall energy is 0.205(9), which is about four times of the π domain wall energy.

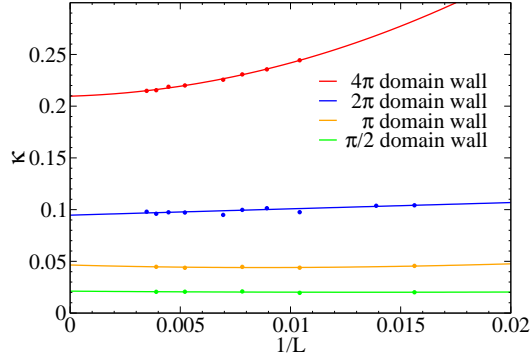


Figure 5. Finite-size scaling analysis of the domain wall energies. The curves are fitted polynomials, used to extrapolate the energies listed in Table 1.

domain wall	$\pi/2$	π	2π	4π
m/N	6	6	4	3
κ	0.0208(5)	0.0434(9)	0.093(9)	0.205(9)

Table 1. Domain wall energy per unit length for various domain walls. m/N is the projection “time” at which the energy is calculated in each case.

4. Summary and Conclusions

Using a ground-state projector QMC method in the VB basis, we have studied projected states in various winding number sectors of the J - Q_3 model on the square lattice. We showed that the projected state stays in the winding number sector of the trial state when system size goes to infinity. The energy of the states in a nontrivial winding number sector have gaps to the VBS ground state in the $W = (0,0)$ sector, due to the presence of domain walls (the winding number counting these domain walls). Such domain walls are stable only for infinite size, thus, the winding number is an emergent quantum number in the thermodynamic limit.

Acknowledgments

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